MST e-NEWS
May 2012

INSIDE

Alison Costello

One for the team

By Diana Del Mauro, ADEPS Communications

Those who don't know Alison Costello by name sometimes refer to her as "The Steelers girl." The team's logo appears on everything from her Los Alamos lanyard to her black-and-yellow purse, not to mention her vast wardrobe of fan apparel.

Alison Costello gives a play-by-play of her work at Los Alamos to Pittsburgh Steeler Franco Harris.
(Photo courtesy of Costello)

The Pittsburgh native has always been a devoted home team girl. But she never imagined that her love for football and her love for science would converge.

Then, in 2009, while at the airport traveling home for Christmas she spied Pittsburgh Steelers' Hall of Famer Franco Harris. Like a "giddy 12-year-old girl," she said she ran over to get his autograph. That's really all she needed, but she was in for a bigger surprise. Harris invited her to sit by him on the plane.

During the plane ride to Pittsburgh, they discussed articles in his copy of *Scientific American*. She never knew he was a science buff. Before they parted ways, Harris jotted down his e-mail address, and Costello invited him to visit her at Los Alamos National Laboratory, where she was a postdoctoral researcher.

Six months later, the former NFL star stood by her side in the actinide research facility, a yellow lab coat draped over his formidable 6-foot-2 frame. It was a day Costello will never forget. They gazed at a glowing uranium compound she had synthesized and placed under an ultraviolet light revealing its characteristics.
"He was just enamored with the place," Costello said.

Last year, when she was made staff scientist on the Surface Science and Corrosion team of Nuclear Materials Science (MST-16), Harris was among the first people Costello told. "He turned out to be a very good friend," she said.

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From David's Desk

Our Worker Safety and Security Teams (WSSTs) are an important part of our safety culture at LANL. Thomas Sisneros (MST-8), the new MST WSST chair, is very enthusiastic about trying to increase the visibility and effectiveness of the MST WSST. One of the primary goals of the WSST is to have MST workers actively identifying safety and security issues in the workplace and helping to resolve them.

The MST WSST has group-level Solutions Teams, which are small teams of workers that go out into the workplace, observe work, and find solutions to improve safety. The Solutions Teams are not in the workplace to audit you. They are there to help you and begin to foster more communication amongst workers about workplace safety. These teams are highly encouraged to fix minor problems on the spot (e.g. labeling, safety glasses, ergonomics, etc.). If the problem requires funding resources, MST-DO has set aside some funds to address issues as they arise. If the issues are large projects with a high cost, then the group offices can work with the MST-DO, ADEPS and FOD to identify funds to correct.

'Our workers are our first line of defense against safety issues.'

Membership on the Solution Teams rotates twice a year, and I highly encourage you to volunteer for one of the rotations. Currently, the MST WSST members and alternates are Diana Honnell and Dave Alexander (MST-6); Thomas Sisneros and Veronica Livescu (MST-8); and Chris Hamilton and Robert Sanchez (MST-7); as well as Glenda Bustos (MST-16), who participates in the TA-55 WSST. Please contact any of these people to get more engaged in worker-based safety efforts. Our workers are our first line of defense against safety issues and you are the ones to identify the best solutions for your work environment.

Lastly, mark your calendars for the WSST Fest on July 10 and visit the MST booth.

MST Division Leader David Teter

Costello . . .

From fan to team player

Team spirit is a big reason why Costello came to Los Alamos in 1996 as a SERS (Science and Engineering Research Semester) student at the Tritium Systems Test Assembly (TSTA) at TA-21. It's also why she returned to Los Alamos as a Seaborg Institute Postdoctoral Fellow in the Chemistry Division nearly a decade later, after completing her PhD in physical inorganic chemistry at the University of New Mexico.

"This environment is about contributing to a larger goal beyond your specific research," she said.

Her interest in spectroscopy, an investigative technique for charting the intensity of light emitted from or absorbed by substances, led her to study plutonium, "one of the most scientifically challenging elements," she said.

"Plutonium is amazingly complex," she said, "because it is a highly reactive metal, making its interaction with other materials unpredictable and exciting."

While deepening the fundamental understanding of plutonium's chemistry and properties, Costello's work also is important for characterizing new and aged nuclear weapon construction materials, such as pits that function as the hearts of weapons. "By having a scientist directly involved in all aspects of the work, from sample selection to performing the experiments to data analysis to publication, a true understanding of the science is possible," her team leader David Moore said.

Preparing tiny pieces of plutonium for an off-site experiment can be as intricate as a football play. The whole team must get involved, including scientists, technicians, and Laboratory shipping and material control staff "to handle all of the technical, safety, and security requirements," Costello said.

For the team's last experiment using high-energy x-rays at California's SLAC National Accelerator Laboratory, Costello was instrumental in coordinating many aspects, from sample preparation to data collection. Radioactive and desirable as a nuclear material, plutonium requires 24-hour monitoring. The experiment required tag teaming to monitor the samples during the experiment as well coordinating the local ES&H (environment, safety, and health) resources.

Scientists at Los Alamos's plutonium facility, for the same security reasons, must be highly dedicated and work in pairs. "Nobody does anything by themselves," Costello said. "It's such a team effort, and that's why I love our group."

Alison Costello's favorite experiment

What: Spectroscopic studies of actinyls (O=U=O, O=Np=O) incorporated into metal-oxygen, polyoxometalate (POM) clusters

Why: To fully understand the electronic structure and bonding properties of actinyls with applications in catalysis and nuclear fuel separation technologies

Who: Alison Costello, (Inorganic, Isotope and Actinide Chemistry, C-IIAC); mentor Iain May (C-IIAC); collaborators Marianne Wilkerson (Nuclear and Radiochemistry, C-NR), John Berg (Manufacturing Engineering and Technology, MET-1), and Steve Conradson (Materials Science in Radiation and Dynamics Extremes, MST-8)

When: 2008-2010, as a G.T. Seaborg Institute Postdoctoral Fellow

Where: TA-48, RC-1, Los Alamos National Laboratory

How: Utilizing an array of spectroscopies, including absorption, emission, Raman and high energy x-rays (EXAFS)

The "a-ha moment:" A series of uranium:POM complexes with subtle structural variances were synthesized. Two years of spectroscopically probing these complexes led to many interesting results. Personally, I was amazed at the degree to which such seemingly minor structural changes resulted in astounding changes in the complexes' properties, including solubility and absorption/ emission. For instance, utilizing sodium (Na^+) as a counter cation produced a complex that was readily soluble in near neutral pH solution. In contrast, incorporation of ammonium (NH_4^+) or potassium (K^+) as the counter cation resulted in a complex that was 10 times less soluble. In addition, one could readily distinguish the Na^+ from the NH_4^+ and K^+ complexes using a simple technique like UV-Vis spectroscopy.

High-energy x-ray diffraction and tomography used to characterize ceramic nuclear fuels

Working with collaborators at Argonne National Laboratory's Advanced Photon Source, Levente Balogh and Stephen Niezgoda (MST-8) recently completed high-energy x-ray diffraction microscopy (HEDM) and micro-tomography (mT) measurements on ceramic nuclear fuel (UO_2) using the 1ID beamline. Microstructural evolution of the ceramic fuel affects the thermal conductivity of the fuel (i.e., the ability to extract heat) and the transport of fission gasses to the fuel cladding interface. Figure 1 shows a picture of a spent fuel pin where cracks and pores are evident, as is the radial

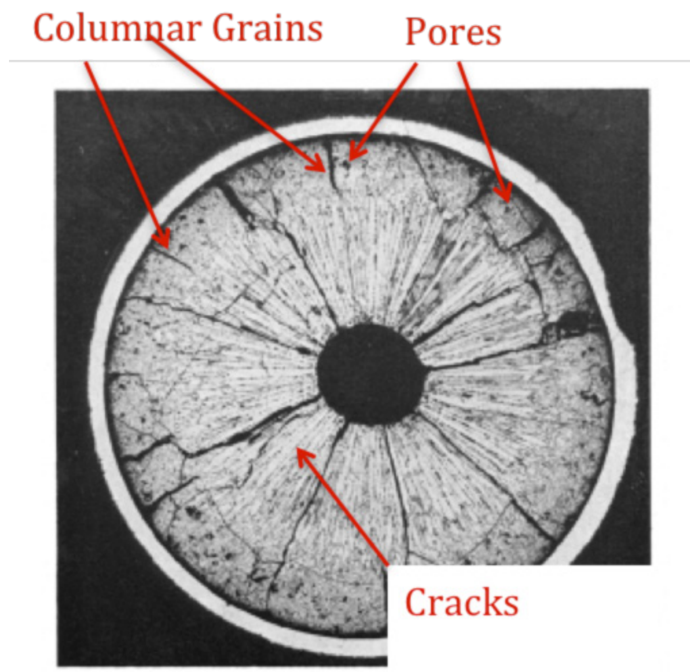

Figure 1. Section thorugh an irradiated fuel pin, showing columnar grains and collection of porosity as a central cavity (x10).

growth of the grains. HEDM and mT allow scientists to characterize exactly these features of the material nondestructively. (Figure 1 is taken from "The Kinetics of Pore Movement in UO_2 Fuel Rods" by P.F. Sens, published in the *Journal of Nuclear Materials*, **43** 293-307 [1972], by North-Holland Publishing Co., Amsterdam.)

Figure 2 shows grain maps collected from a ceramic nuclear fuel sample using HEDM. It is important to note that this map represents grains in the bulk of the sample, not on the surface, and that the measurements were completed nondestructively and with little or no sample preparation, saving costly and hazardous sample handling.

From this data special grain boundaries from within coincident site lattice theory may be identified. Since the measurement is nondestructive, one can imagine secondary measurements, for instance, after a thermal cycle similar to that experienced *in-operato*, during which the grains grow in the direction of a thermal gradient. This second measurement and associated analysis will allow this research team to determine which grain boundary types are most favored for growth, which feeds directly into theoretical work attempting to predict the microstructural evolution of fuel pellets.

To the right of Figure 2 is a computed tomograph of the same sample. Pores in the size range from a few to tens of microns are evident. Improvements to the experimental system will offer a 2X or more improvement in resolution. Again, because the measurement is nondestructive, this research team envisions repeating these

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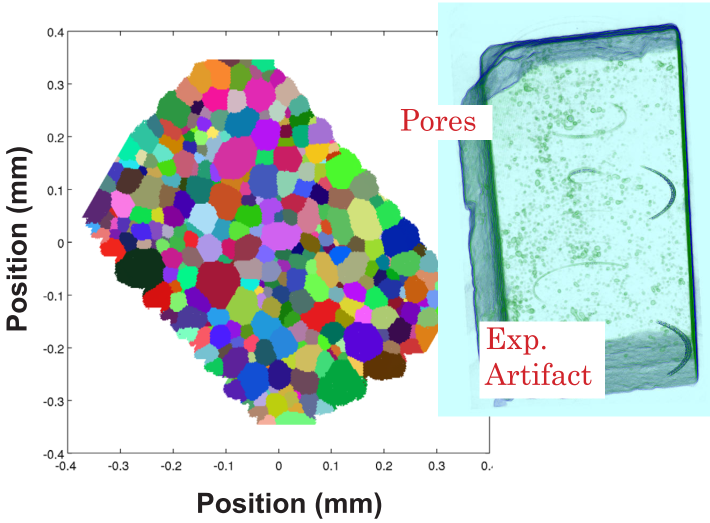

Figure 2.

Fuels. . . measurements on single samples at multiple stages, such as before and after sintering, or before and after an accident scenario to characterize the evolution of the pores and/or cracks under these conditions.

The urania (UO_2) sample was fabricated by Darrin Byler and Ken McClellan (MST-8) and Andy Nelson (Polymers and Coatings, MST-7). James Hunter of Applied Engineering and Technology (AET-6) and Chris Hefferan of Carnegie Mellon University assisted in data analysis. The work was funded by LDRD.

Technical contacts: Levente Balogh and Don Brown

MST researchers unravel cause of lattice swelling in complex oxides

In fundamental research that could lead to a better understanding of why some materials are more radiation resistant than others, Materials Science and Technology researchers and external collaborators explored a phenomenon of both scientific and practical importance–the swelling of crystalline solids due to radiation damage.

The findings, accepted for publication by *Physical Review Letters*, have implications not only for radiation damage effects in complex oxides, but also for oxygen transport in solid oxide fuel cells and for thermal transport in inert matrix fuels and thermal barrier coatings.

The work demonstrates experimental evidence for a correlation between irradiation-induced atomic disorder and lattice swelling in a ceramic oxide pyrochlore-structured compound, $Lu_2Ti_2O_7$ (LTO), with supporting theoretical evidence for the nature of the defects responsible for this swelling.

Starting with polycrystalline, monophasic samples of LTO, the scientists fashioned cut-and-polished disks. Using the Danfysik ion implanter in the Ion Beam Materials Laboratory, they irradiated the disks with 400 keV Ne^{2+} ions at cryogenic temperature (~77 K). Then, using x-ray diffraction, they examined the LTO samples before and after irradiation.

Three pieces of evidence, both experimental and theoretical, collectively revealed that titanate pyrochlores experience significant radiation-induced swelling at low displacement damage doses, and that this swelling is due explicitly to the formation of cation disorder defects.

Though disordering studies have been done since 1936, the detailed contributions of defects to lattice swelling have not been well understood. In this paper, the researchers determined that the swelling was due to the *antisite* defect. Antisite defects occur in pyrochlore when atoms on one cation sublattice exchange positions with atoms on the other cation sublattice, forming antisites.

The researchers concluded that the formation of antisites, observed in the experiment, must occur "in-cascade," as energetic displaced atoms thermalize following cascade events. Atomistic simulations, using accelerated molecular dynamics, showed that the barriers are much higher for neighboring antisites to annihilate and produce perfect crystal (>10 eV), meaning that once they form, they will be stable for extremely long times. The fact that antisites are observed in the experiment leads to the conclusion that they must then have formed in-cascade.

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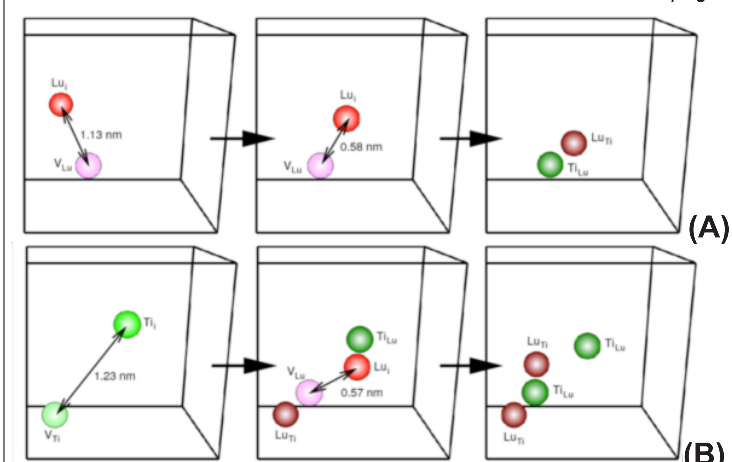

Frames from temperature accelerated dynamics simulations showing the evolution of point defects in $Lu_2Ti_2O_7$. (A) Lu Frenkel pair ($Lu_i + V_{Lu}$). The Lu_i and V_{Lu} point defects migrate towards one another, but rather than annihilating to produce perfect crystal, they decay into a near-neighbor antisite pair ($Lu_{Ti} + Ti_{Lu}$). (B) Ti Frenkel pair ($Tii + V_{Ti}$). The Tii does not migrate, but instead decays into the defect pair, $Lu_i + Ti_{Lu}$. V_{Ti} also decays during migration into an additional defect pair, $V_{Lu} + Lu_{Ti}$. The $Lu_i + V_{Lu}$ defects then react as in (A), leaving two antisite pairs ($Lu_{Ti} + Ti_{Lu}$).

Swelling... Los Alamos researchers from MST-8 include: Y. H. Li (also of Lanzhou University, China), B. P. Uberuaga, C. Jiang, (now at University of Wisconsin, Madison), S. Choudhury, J. A. Valdez, M. K. Patel, J. Won, Y.-Q. Wang, M. Tang, D. D. Byler, K. J. McClellan, and K. E. Sickafus (now head of Materials at University of Tennessee, Knoxville); from Materials Technology-Metallurgy, MST-6, D. J. Safarik; and from Polymers & Coatings, MST-7, I. O. Usov.

The DOE Office of Basic Energy Sciences, Division of Materials Sciences funded the Los Alamos portion of the work. The research is tied to the Materials for the Future science pillar and the Nuclear Deterrence, Global Security, and Energy Security mission areas.

Technical Contact: Blas Uberuaga

Measuring Poisson ratio for poly(siloxane) foams in compression

Researchers in Polymers and Coatings (MST-7) have successfully measured for the first time the Poisson ratio for poly(siloxane) foams in compression using micro x-ray computed tomography. The Poisson ratio is a measure of the transverse strain (expansion of a material lateral to the direction of compression) to the amount of stress (compression). For most solid materials, the Poisson ratio is a single positive value, for foams, the ratio increases with compression, becoming a steady state value when the foam is at full density. Some materials, such as paper, become thinner when compressed (a negative Poisson ratio), and a few materials do not expand when compressed (auxetic) such as cork, they have a Poisson ratio of zero. Measuring the Poisson ratio for foams (polymeric or metallic) is especially difficult due to the fact that the Poisson ration changes as stress is applied to higher loads. Also, materials respond to that stress in three dimensions, almost requiring a 3D technique to measure. Using MXCT, foam samples are imaged in a compression cell uncompressed, and then again after compressing sequentially to higher and higher applied stress (Figure 3). In this figure, the waist of the material is moving from a concave to a convex geometry. From these 3D images a measure of the radius (strain) of the waist can be taken by fitting a circle. Plotting the Poisson ratio versus the percent strain (Figure 4) graphically displays the change in the Poisson ratio with compression. Due to the difficulty in acquiring this type of information, until now, the Poisson ratio has not been known for this material.

Two formulations of poly(siloxane) foams, SX462 (pristine and thermally aged in an oven at 70 ^{o}C for 6 months) and pristine SX358 were imaged in this manner and their Poisson ratio's

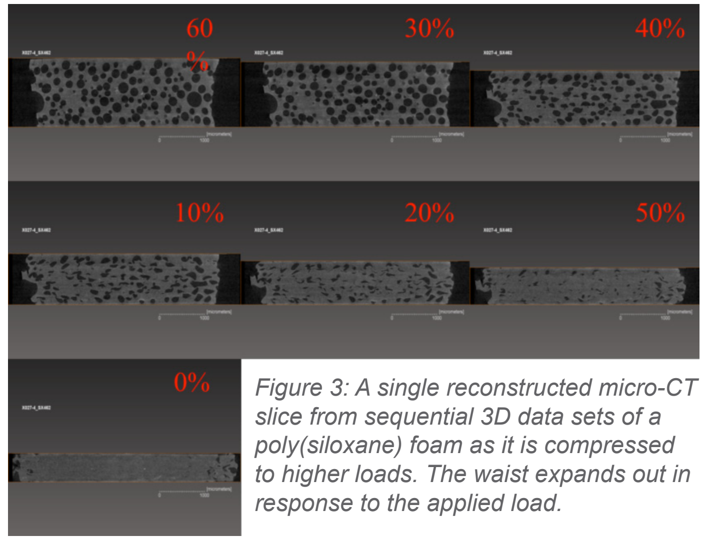

Figure 3: A single reconstructed micro-CT slice from sequential 3D data sets of a poly(siloxane) foam as it is compressed to higher loads. The waist expands out in response to the applied load.

measured. SX358 (60.5% void volume) and SX462 (42.9% void volume) vary slightly in their formulations. Both are filled, hydrogen-blown, polydimethylsiloxane(PDMS)-based materials cross-linked by polymethylhydrosilane (PMHS) and tetrapropylorthosilicate (TPOS). SX462 contains more PMHS, which bonds to the ends of the PDMS backbone. The molecular weight distribution of PDMS in SX462 also includes more of the larger chains than SX358. These two differences are expected to influence both elastic properties and microstructure. The Poisson ratio has a significant effect on the results of dynamic engineering models for weapon systems. Characterization of the Poisson ratio is expected to improve model predictions.

Future work will focus on repeating these measures for a multitude of pristine and aged (thermally, irradiated) materials as well as for samples of various sizes. This work was completed by MST-7 personnel Brian M. Patterson, Kevin Henderson, Zachary Smith and Steve Birdsell (Enhanced Surveillance NNM Project Leader) and was funded by the Enhanced Surveillance Program (Tom Zocco, Program Manager) and Campaign 2 (Rick Martineau, Program Manager).

Technical contact: Brian M. Patterson

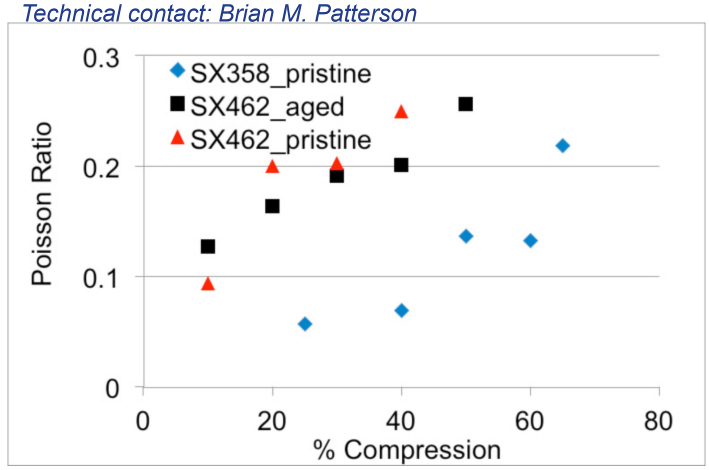

Figure 4: Poisson ratio of the three poly(siloxane) foams. The two formulations show different Poisson ratio's, with the pristine and aged SX462 only showing a slight change in slope.

Clarke recognized with early career research award

Amy Clarke of Materials Technology (MST-6) is the recipient of a DOE Office of Science 2012 Early Career Award.

The DOE Office of Science recently announced the researchers who have been selected for a financial award under the fiscal year 2012 Early Career Research program. The funding opportunity for researchers in universities and DOE national laboratories supports the development of individual research programs of outstanding scientists early in their careers and stimulates research careers in the disciplines supported by the Office of Science.

Clarke's award project, "In situ Monitoring of Dynamic Phenomena during Solidification," focuses on the ability to visualize experimentally and model theoretically the melting and solidification processes of metal alloy materials, even at elevated temperatures. The project will use novel tools and unique probes, such as synchrotron x-ray and proton radiography and tomography, at national laboratory facilities that have not yet been used in the United States for this purpose. Modeling these processes will enable the prediction of the microscopic structure of metal alloys, even under harsh environments and will enable new understanding of a range of energy materials, such as wind turbine blades and lithium rechargeable batteries. Clarke received a doctorate in metallurgical and materials engineering from the Colorado School of Mines. She is a former Seaborg Institute postdoctoral fellow at Los Alamos and a recipient of The Minerals, Metals & Materials Society (TMS) Young Leaders Professional Development Award.

The mission of the Office of Science is to deliver scientific discoveries and major scientific tools to transform the understanding of nature and to advance the energy, economic, and national security of the United States. The Office of Science gives Early Career Awards in the following program areas: Advanced Scientific Computing Research (ASCR), Biological and Environmental Research (BER), Basic Energy Sciences (BES), Fusion Energy Sciences (FES); High Energy Physics (HEP), and Nuclear Physics (NP). Recipients of the Early Career Awards are within 10 years of having received a doctorate and are either untenured assistant professors on the tenure track, untenured associate professors on the tenure track, or full-time, nonpostdoctoral, permanent DOE national laboratory employees. The 68 recipients for fiscal year 2012 were chosen based on peer review of about 850 proposals.

2012 Materials Capability Review Committee

Members from left: Barbara Jones, vice-chair, IBM Research; Gary Was, chair, University of Michigan; Christine Orme, Lawrence Livermore National Laboratory; Richard LeSar, Iowa State University; Thomas Russell, Air Force Office of Scientific Research; Robbie Vogt, LANS Science and Technology Committee representative, California Institute of Technology; Alexandra Navrotsky, LANS Science and Technology Committee representative, University of California, Davis; Robert Powell, University of California observer; Jeffrey Lynn, National Institute of Standards and Technology; Dmitri Bassov, University of California San Diego; Michael Kaufman, Colorado School of Mines.

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries this month:

Joni Powell, MST-6	35 years
Robert Dickerson, MST-6	15 years
Joseph Anderson, MST-16	10 years
Wanda Duncan, MST-16	10 years
Andrew Nelson, MST-7	5 years

MST e NEWS

Published monthly by the Experimental Physical Sciences Directorate.
To submit news items or for more information, contact Karen Kippen, EPS Communications, at 606-1822, or kkippen@lanl.gov.

LALP-12-007
To read past issues, please see www.lanl.gov/orgs/mst/mst_enews.shtml.

Los Alamos NATIONAL LABORATORY EST. 1943

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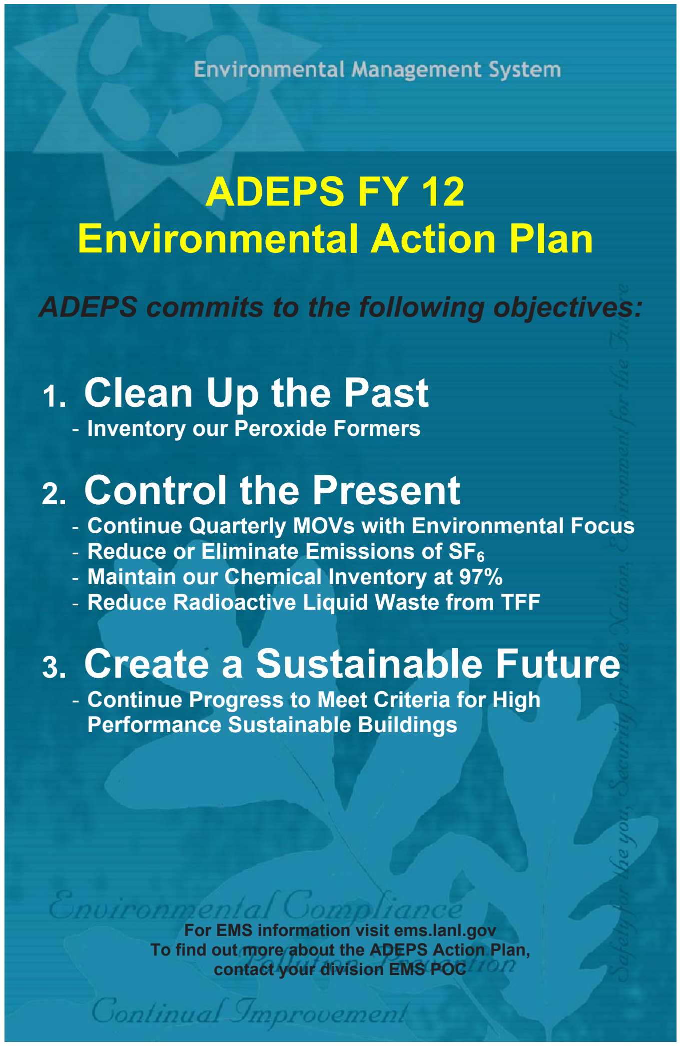
It's time to come up to speed on the Directorate's implementation of the FY12 Environmental Action Plan (EAP) that was developed in support of the Lab's Environmental Management System. The ADEPS team responsible for developing and disseminating the plan includes Steve Glick from P Division (also serves as the Directorate Point of Contact), Jim Coy from MST, Cathy Padró from MPA, and Frances Aull from LANSCE.



Our 2012 Environmental Action Plan addresses our impact on the environment. You have seen the poster: we will attack this from three angles—the past, the present, and the future.

Let's look at our objectives, and the specific targets we have developed to meet the objectives. These objectives parallel the LANL institutional objectives, with the targets fine-tuned to fit our Directorate's needs.

Objective 1 – Reduce Environmental Risks from Historical Operations, Legacy, and Excess Materials and Other Conditions Associated with Activities No Longer a Part of Current Operations (CLEAN UP THE PAST). Last year, we worked with the Lab's Environmental Team to understand our chemical waste generation profile so that we can establish long-term waste-reduction goals. Our focus this year is peroxide formers—we will perform a focused inventory of out-of-date peroxide formers to ensure proper testing and to identify potential disposal pathways.

Objective 2: Control and Reduce Environmental Risks from Current, Ongoing Operations, Mission, and Work Scope (CONTROL THE PRESENT). Managers will continue to emphasize environmental aspects during MOVs, we will conduct an annual chemical inventory, and we will disseminate information on the EAP using posters, group briefings, and e-mails. In addition, we are specifically targeting reduction or elimination of SF_6 releases. SF_6 is an extremely potent greenhouse gas and reducing or eliminating emissions is an institutional goal associated with the Site Sustainability Plan. Finally, MST Division was in line to receive institutional funding to reroute non-RLW (rad liquid waste) discharges at Target Fab Facility that currently go to the RLW Treatment Facility, but the project is on hold due to the funding being withdrawn.

Objective 3 – Reduce Environmental Risk from Customer Expectations and Regulatory Requirements Associated with Future Conditions, Managing these in Alignment with Short- and Long-Term Planning, Work Scope Projects, etc. (CREATE A SUSTAINABLE FUTURE). We will continue to work towards the requirements for High-Efficiency Sustainable Building recognition for the MS-OB (03-1415), including additional tenant education and the formation of a Green Team.

To succeed, we need everyone to "up" their awareness and take action. Turn off lights in offices, conference rooms, hallways, and labs when not in use. Get that leaking faucet/toilet/urinal fixed (contact your facilities coordinator). Turn off computer peripherals when not in use. Alter your purchasing habits–Purchase GREEN. Use the blue and green recycling bins. Share chemicals, minimize chemical inventories, purchase safer alternatives, recycle and dispose properly. Salvage all unnecessary or unused (and not needed) equipment. Nominate a deserving colleague for a P2 (Pollution Prevention) Award!!

Document, Record & Report all significant environmental actions that you take that positively affect the environment. Remember, if it's not recorded, it didn't happen. Please send your environmental action reports (e-mails are fine) to your Division contact: jcoy@lanl.gov for MST; padro@lanl.gov for MPA; aull@lanl.gov for LANSCE, and sglick@lanl.gov for P Division. This will ensure that our efforts continue to get the deserved recognition for our environmental efforts.

Steve Glick, ADEPS EMS point of contact